Pharmacological Analogues of Erinacine A and Hericenones from *Hericium erinaceus*: Rational Design of Non-Psychedelic Neurotrophic, Nootropic, Antidepressant, Synaptogenic, Myelinogenic, Geroprotective and Telomerase-Activating Agents

Yaroslav Grigorievich Zaitsev ORCID: 0000-0002-0069-2997

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Abstract

Erinacine A and hericenones from *Hericium erinaceus* are among the most potent known inducers of nerve growth factor (NGF) capable of crossing the blood-brain barrier. This work presents 52 simplified hybrid analogues combining key pharmacophores of erinacine A (pro-indole tryptamine motif, cycloheptane-derived fragments) and hericenones (lipophilic isoprenoid domain) with ultra-lipophilic scaffolds derived from carvacrol, α/β-asarone, reduced tryptophols and related structures. The designs exploit ultra-low-affinity, thermal-fluctuation-assisted receptor activation via deep membrane partitioning, delivering sustained "slow neuroplasticity" without psychedelic effects or 5-HT_2B risk. Predicted logP 4.4–6.8, MW < 550 Da, synthetic accessibility 1–4 steps. The analogues aim to overcome the limitations of natural compounds while preserving and enhancing neurotrophic, antidepressant, synaptogenic, myelinogenic and geroprotective activity.

Keywords: erinacine A analogues, hericenones, *Hericium erinaceus*, neurotrophic agents, rational drug design, non-psychedelic neuroplasticity, slow neuroplasticity, lipophilic 5-HT_2B mimetics, NGF/BDNF inducers, telomerase modulation, geroprotectors

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1. Introduction

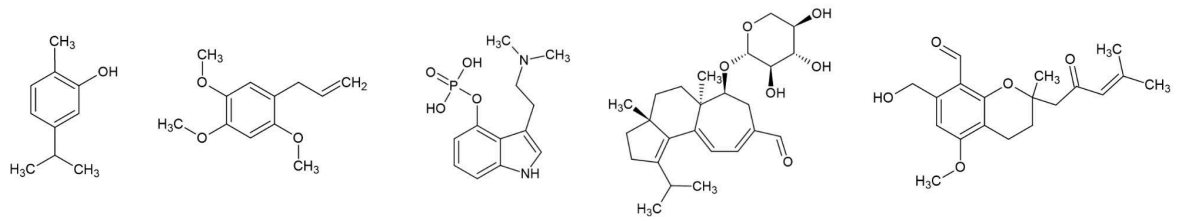

Figure 1. Reference compounds: Carvacrol – α/β-Asarone – Psilocybin – Erinacine A – Hericenones

Erinacine A and psilocybin exhibit partially overlapping pharmacological profiles, yet differ significantly in speed and safety. Like psilocybin, erinacine A possesses a pro-indole structure and contains a special hydrophilic ligand (glycoside radical vs phosphate in psilocybin). Its cycloheptane ring equipped with aldehyde and alcoholic hydroxyl groups is likely capable of pro-serotonergic activity both independently and within a terpenoid framework. The isopropyl radical of erinacine A and the structurally similar carvacrol motif further contribute to this activity.

The markedly more lipophilic and non-psychedelic profile of erinacine A and hericenones confers a major advantage over classical psychedelics and dissociatives. Erinacine A acts as a slow neuroplastic agent with deeper, more constructive mechanisms compared to rapid-acting antidepressants or psychedelics.

Rapid neuroplasticity (psilocybin, ketamine) promotes enhanced synaptogenesis, but can duplicate pathological connections and increase neuronal noise. In contrast, slow neuroplasticity — true neurogenesis and myelinogenesis — appears preferable for organic brain lesions, depression, Alzheimer's disease and related conditions.

Psilocybin has also been shown to extend replicative lifespan by up to 50% via telomerase modulation and reduction of oxidative stress. Combined neurotrophic, nootropic, synaptogenic, myelinogenic, neuroprotective and lifespan-extending effects make erinacine A and hericenones ideal templates for next-generation therapeutic agents.

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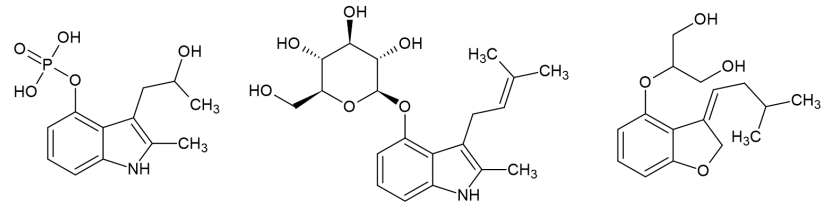
2. Rationale and Proposed Structures

Hericenones and erinacine A exhibit exceptionally high lipophilicity and the ability to stimulate intracellular allosteric serotonin centres. α/β-Asarone and carvacrol display similar neurotrophic/antidepressant properties and excellent brain penetration. These scaffolds were therefore selected as the foundation for hybrid design.

Figure 2.

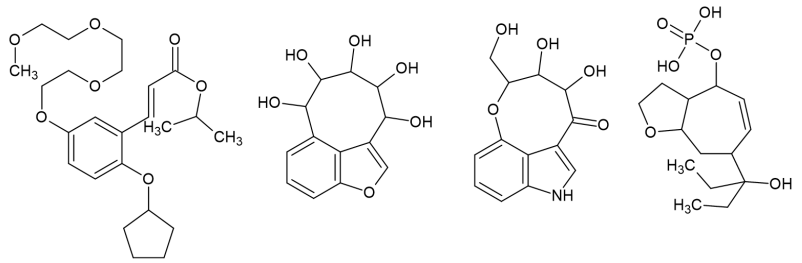


Row 1

1.1 A lipophilic tryptophol with reduced psychoactivity (2-methyl group). It contains a hydroxyl group mimetic of the amino group and contains the entire spectrum of pharmacophores necessary for pro-serotonergic activity. For prodrug potential and hydrophilicity, it contains a phosphate residue - a more complex version of the simplest core.

1.2 A variant is shown substituting tryptophol with its diene analog, which has an even lower affinity, dipole moment compared to hydroxyls as analogs of the amino group of tryptophols. However, the glycoside group hints at the hydroxyl nature of the prodrug and some hydroxyl accumulation in the working zone, which may somewhat activate direct mimetic properties in the future development of similar structures.

1.3 The structure contains a furan ring, departs from the toxicology of indoles, isopropyl similar to Erinacins is directed in the plane as in indole, activation occurs by a double bond and hydroxyls located in the active zone.



Row 2

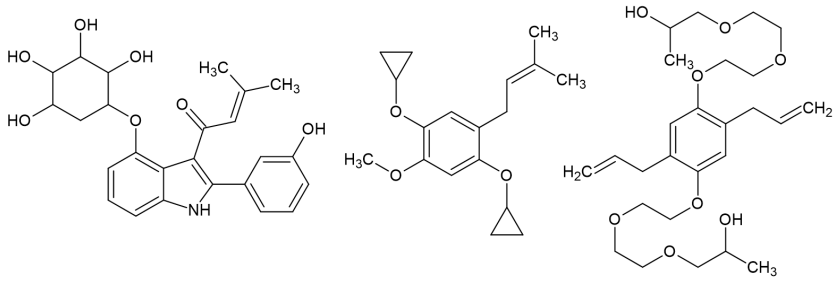
2.1 Cinnamic acid derivative, removal of the indole ring, and search for non-oxidative, lipophilic, and rapidly catabolized rings where the ester is shortest-lived. The ester bond of cinnamic acid derivatives produces a strong enolic effect, sufficient for subtle mimetic activity, such as the amino group of serotonin or the hydroxyl group of tryptophols. Cinnamic acid does not require a displacing radical at the para position, since the ketone group of the ester group is located in the active site of the serotonin amino group. Meta-methoxyl or simple ester groups mime the 5-hydroxyl group of serotonin, while ortho-methoxyl or cyclopentoxyl groups mime the indole pentagonal ring and the neutral nitrogen of the indole. There is a possibility of para-catechin formation, but the sequence of metabolic reactions and the rate of metabolism of the substance provide a good prognosis for the high safety of the substance.

2.2 A furan analogue of serotonin with a 5-hydroxy radical actuator at the 4-position, multiple hydroxyl groups for increased hydrophilicity, enhanced catabolism, and blurring of the

powerful actuator—the hydroxy group, the multiple repetition of which creates a multi-readable, sterically hindered, less active variation.

2.3 A variation of core 2, but in an indole version, in which part of the glycoside is stabilized by a cyclic conformation, duplicating multiple hydroxyls in the active zone of the amino group of serotonin and pointing to the hydroxyl at the 4-position, which makes the structure less amenable to indole-metabolizing enzymes.

2.4 The structure contains a complex terpenoid lipophilic core with an inverted indole component and similar to some powerful synthetic neuroplastic substances and Erinacine. It is also available as a more hydrophilic formulation of the drug to provide a wider range of dosage forms.



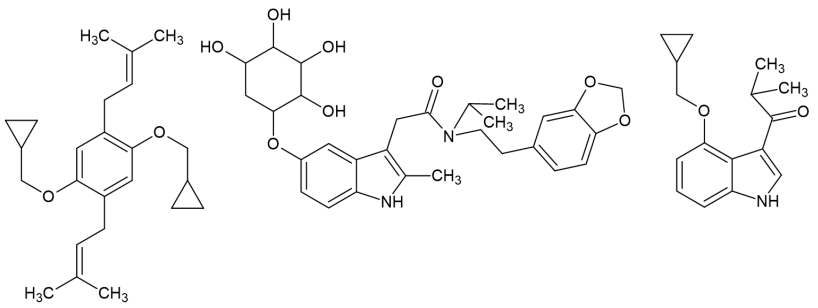
Row 3

3.1 A substance of indole nature, with a powerful substituent that blocks psychoactivity, inhibits enzymes that metabolize indoles, and creates a dual reading of serotonin. Since the phenol at the second position of the indole is located within the aromatic ring of indole-serotonin, when reading the structure from the direction of the phenol and moving the diene substituent toward it, a dual reading of the indole is created. The diene group is also activated by the keto group, and the isopropyl radical subtly emphasizes the mimetic properties of serotonin, bufotenine, and DMT.

3.2 A hybrid compound of asarone, eugenol, and erinacin, multiplied by several special readings. The methoxy substituent is a repulsive one, enlarging the aromatic ring, making it mimetic for pro-serotonin activity. Alkyl cyclopropane groups in the ortho position mimic the indole moiety, while in the meta position, they mimic the 5-hydroxy group of serotonin. Furthermore, cyclopropane radicals, having special banana bonds stimulating hydrophilic behavior, duplicate the pro-amino group when the molecule is read at other angles. Thus, the structure contains both lipophilic pro-ethylamine sites and more hydrophilic duplicate sites in the working region and can be sorbed onto various types of receptors and allosteric sites, selecting the affinity configuration for different topologies. Simultaneous dynamic effects on multiple receptors are also possible. Because activity relative to asarone can increase sharply, and dealkylation and formation of para-catechins may have a different sequence, the substance is at risk for carcinogenic effects, but has the potential to escape this risk through a simple tautomeric design. High lipophilicity and metabolic potential may provide good pharmacodynamics for such a simple structure.

3.3 A substance that transitions from eugenol to asarone has two reading directions and may be much more active. Methoxyl or polyether groups universally mimic the 5-hydroxy

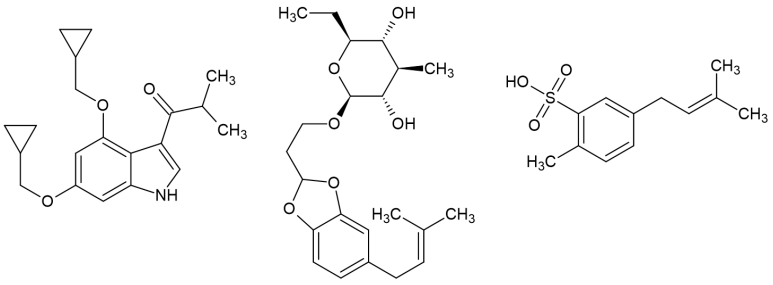
group and indole nitrogen. In this embodiment, the polyether groups may impart a unique pharmacological profile and also act as a duplicate of the pro-hydroxyl mimetic dipole moments of allyl radicals. The pharmacokinetics of such substances can be regulated by polyether groups; the danger of para-pyrocatechins remains questionable.



Row 4

4.2 A lipophilic amide, indole, catecholamine, and n-BOM ultra-light mimetic with a protective indole methyl group at position-2, minimal affinity for the serotonin amino group, a maximally extended bioavailable configuration, and a pronounced hydrophilic component in the form of a stable pro-fungal glycoside. The substance contains various reading variants, has fairly good bioavailability of the main core, and is equipped with many specific radicals that can cause a certain selectivity for receptors and allosteric sites.

4.3 The simplest indole configuration, biostabilized and activated by a radical at the 4-position, simple and pure pharmacological organic synthesis, good starting toxicological positions, some dual activation of ethylamine mimesis using keto-substituents and cyclopropane hydrophilic action.

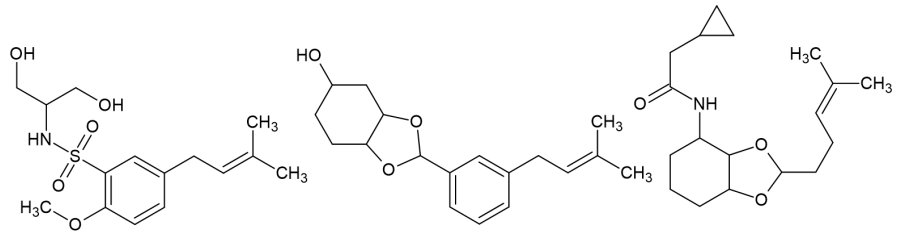


Row 5

5.1 A modified core from the previous line. The additional cyclopropanemethoxy group suggests a potential reduction in indole activity, but also a special reading on the reverse side. The inverted reading may enhance activation of certain targets associated with active neuronal growth factors. The dual reading may also activate more receptors with a specific landscape.

5.2 A non-indole variation of the dual reading of serotonin with a pattern inversion similar to the previous structure. Contains a glycosidic radical.

5.3 A derivative close to carvacrol, with elements of erinacine, a special sulfonamide group, which may be a special tactical device in the drug design of such compounds.

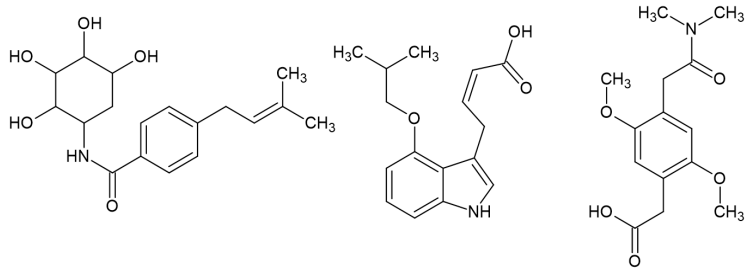


Row 6

6.1 A variant of the sulfamide group, the paramethoxy group acts as a displacer and directs activity toward the pro-serotonin side; the dimethylallyl radical subtly but clearly indicates the ethylamine group in serotonin and bufotinin; and the sulfamide group, together with additional hydroxyl radicals, creates a substituent at the 5-position and a special hydrophilic shell near the working zone, as well as unique metabolism and pharmacokinetics.

6.2 A dioxolane prototype with a dual serotonin nature, realized on the unsaturated core and the aromatic core. The unsaturated core is bulky and, being in the meta position, has the ability to serve as a displacer to enhance the pro-serotonin affinity of the aromatic core. The saturated core also has a pro-serotonin structure and is capable of complementing various sites dynamically.

6.3 An aliphatic pro-serotonin mimetic, built on a short-lived dioxolane bridge that realizes an isoindole projection of the structure. The unsaturated dipole pro-amine tail is duplicated by a special amide radical with the pro-hydroxyl potential of cyclopropane.



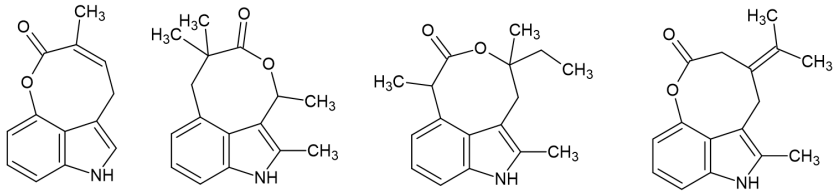
Row 7

7.1 A dimethyl allyl radical with a displacing radical—a carboxylic amide—is a special form of a stable mushroom glycoside analogue, converting the substance into a soluble form and donating a hydroxyl group at a position close to the 5-hydroxy group of serotonin.

7.2 Can an acid deceive the receptor? This is precisely the question posed by this substance. Yes, the carboxyl group can reduce the ability to mimetic serotonin, but two readings of this molecule offer the possibility of agonist or agonist-antagonist potential, which in turn may be a useful configuration for the search for specific, selective, and subtle

activators of neurogenesis. Ease of synthesis also offers high safety and a number of unique physicochemical and pharmacokinetic properties.

7.3 The same principle as the previous structure, but implemented on an aromatic core; the acetic residue in this structure acts as both a core displacing agent and an antagonist. In this case, the core is read differently on both sides, but there are options when both sides contain amide groups or these groups contain different radicals, realizing a range of multifaceted capabilities. The danger of para-pyrocatechinization is relative, the nucleus provokes the formation of para-catechins, but the order of reactions and the final catabolites can have a completely different toxicology than in the case of asarone.



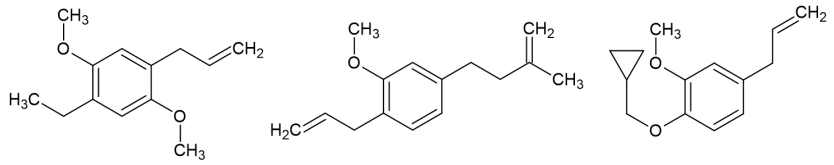
Row 8

8.1 A lactone biostabilized by a hydroxy group at the 4-position has an open carboxyl group, but this is dynamically open, with the potential to convert to the lactone form. The core exhibits a pro-serotonin construct, the active zone of which contains pro-ammine dipole double bonds, methyl, and, slightly to the side, an enolic ketone radical. The substance is lipophilic, bioavailable, and biostable due to the hydroxyl group and the cinnamic diene located next to the keto group.

8.2 A lactone of a completely different nature, a derivative of carboxymethyl indole, with a methyl at the 2-position, which reduces the direct mimetic properties of the alcohol groups. The alcohol group is closed into a lactone, which adds a keto group at the serotonin amino group position and affinity methyls of bufotenin, which are transferred to the 4-position by a substituent, hinting at the 5-hydroxyl of bufotenin. A complex and subtle interplay of mimetic and dynamic properties, a unique profile – unique pharmacology.

8.3 A lactone with a more pronounced tryptophol profile, with reduced psychoactivity due to methylation at the 2-position.

8.4 An analog of the first substance in the series, the lactone is inactive, merely opening access to the hydroxyl at the 4-position. The radical mimetic of ethylamine and dimethylethylamine is pronounced, but particularly subtle and inactive, being a continuation of the allyl radical of asarone, as in many previous structures. While remaining lipophilic, lactones can become hydrophilic; while remaining bioinert, lactones can be easily bound and removed from the lipid layers of tissues; this is the interplay of lipophilic structures in bioavailability and correct pharmacokinetics.

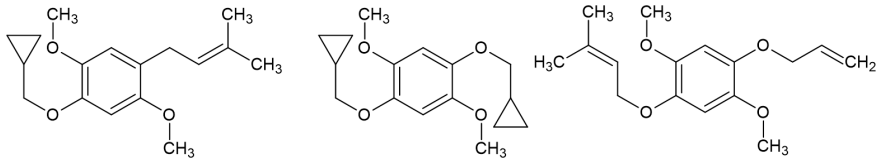


Row 9

9.1 A simple asarone derivative, likely much more lipophilic and active, but with the potential to form para-catechins.

9.2 A compound with a special substituent; the core combines the pharmacology of carvacrol, asarone, and eugenol, reducing the likelihood of para-catechin formation and enabling dual asymmetric reading, dynamic self-complementation, affinity for multiple receptors, high lipophilicity, and possible safety.

9.3 A simple eugenol derivative, synthesized in a single step, but radically altering its pharmacology. The allyl radical now acts as a substituent at the para position, and the cyclopropane alkyl acts as a pro-ethylamine mimetic radical, with the methoxy group acting as the nitrogen atom of indole serotonin. In dynamic thermal motion on the receptor, such a structure can complement itself by rotating in the initiated semi-compressed configuration of the receptor.

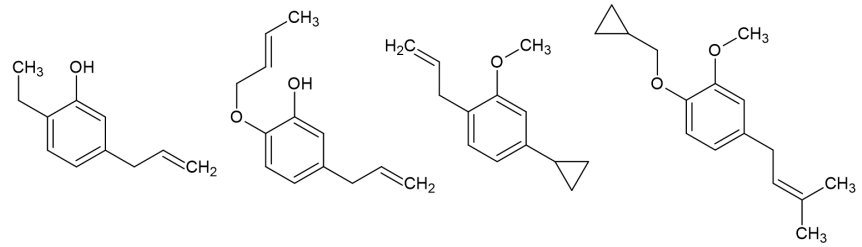


Row 10

10.1 An asarone derivative with two variants of the serotonin sequence may be more active, have a broader spectrum of activity, and a different order of pyracatechinization.

10.2 Departure from the asarone ring, resulting in different pyracatechinization products.

10.3 Special radicals and departure from the asarone ring, similar phenols, allow for two or more interchangeable but distinct radicals. If necessary, the number of tautomers can be increased to tens or hundreds. Moreover, this may be a unique route to obtaining a substance with a broad spectrum of activity at serotonin receptors and allosteric sites. Catabolism is non-reduced, lipophilicity remains high, and safety may be unexpectedly high.



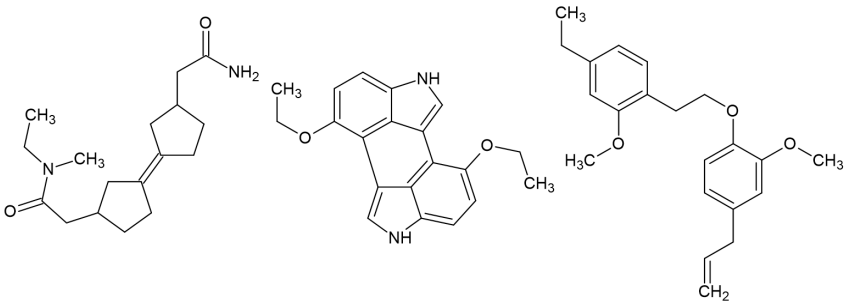
Row 11

11.1 A simple derivative of carvacrol, more lipophilic, more pro-serotonin, closer to asarone, but does not produce carcinogenic pyrocatechols.

11.2 A derivative similar to the first, but with more lipophilic substituents, a possibly two-sided serotonin reading, and a good safety profile.

11.3 A special, complex configuration of carvacrol, asarone, and a new independent nucleus. A two-sided pro-serotonin configuration, the allyl group acts as an ethylamine mimetic radical and as a displacing radical. Cyclopropane also acts as both a displacing radical and an ethyl-proamine radical, but also as a cyclic displacing radical, creating the effect of an inverse indole. The methoxy group, depending on the reading, plays the role of the indole nitrogen, or the 5-hydroxyl of serotonin. A complex and unique highly lipophilic structure that can be not only extremely compact, but also extremely active and multifaceted.

11.4 Eugenol variation, dual activity, dynamic activity, alkylated tautomer of eugenol, completely changing the properties of the original natural substance, in addition to safety and ease of production.



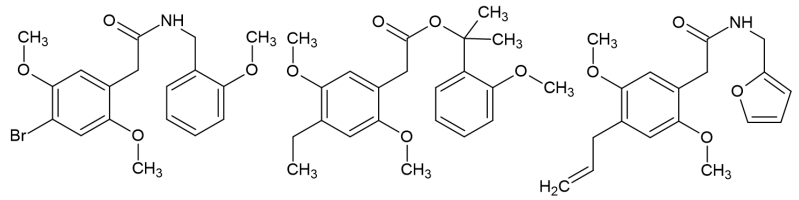
Row 12

12.1 Cyclopentanes fused with a double group are very similar to indole, more biostable, and more subtle as affinity agents. The core is highly lipophilic, and given the two acetic acid groups and the ability to easily obtain various amide mixtures, the core may be a potential candidate for an inert and safe multifunctional drug.

12.2 Condensed indoles, a special topic for theoretical and practical chemistry, are distant indole analogs of hypericin. These substances can block serotonin-catabolism enzymes and

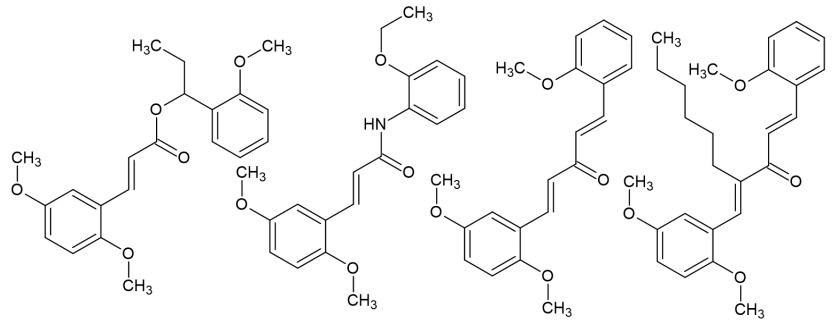
MAO, but also act as subtle mimetics, particularly lipophilic and highly active neurotrophic antidepressants.

12.3 The dual structure, pro-serotonin, which is converted to proserotonin, both parts of the molecule complement each other through the specific placement of methoxyl groups, which eliminates the risk of para-catechin formation. At the same time, both subunits embody different patterns and different types of mimetics of the ethylamine fragment, being to some extent a pharmacological analogy of the previous substance, unfolded into a chain.



Row 13

13.1, 13.2, 13.3 From powerful psychedelics to subtle examples of lipophilicity and activity, from simple analogs to more subtle pro-serotonin derivatives. The first transitional structures, but with great potential.



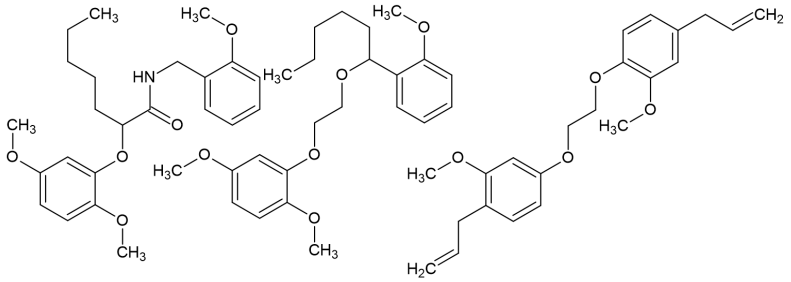
Row 14

14.1 Now, subtle and lipophilic derivatives of potent psychedelics do not require halogenation; their geometry is adjusted without a displacement radical through the use of cinnamic acid derivatives. Such derivatives may not only be more active and therefore carry fewer catechin risks, but also be safer due to the acidic residue of the metabolites. The ester is lipophilic, conditionally bioinert, but relatively rapidly inactivated, demonstrating unique pharmacokinetics.

14.2 The amide variant is more biostable, with a longer half-life.

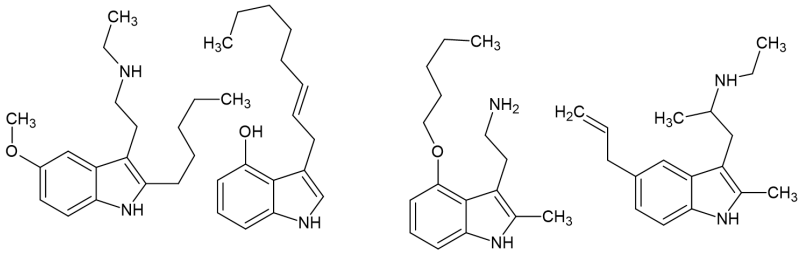
14.3, 14.4 Variants of the croton-condensed nuclei have a special enolic pro-ethylamine radical, a special double pro-serotonin semiflexible structure, as well as special long radicals that can steer mimetic activity toward particularly potent neuronal growth factors. Such condensed structures can also exhibit cannabinoid activity, primarily CB-2 and some others. These structures are a special example of lipophilic condensed active substances with slow

catabolism. They require careful handling and carry an increased risk of incorrect pharmacokinetics, but can also be an excellent configuration for producing prolonged-release, highly active drugs at all levels of biomaterial penetration. Despite the complexity of the pharmacology of this group of substances, the organic synthesis of such derivatives is simple, and the synthesis of condensed structures is also easily achieved by crotonic condensation.



Row 15

15.1–15.4 This line is characterized by a greater emphasis on mimetics of powerful neuronal growth factors than the previous one. It also features a unique multi-component design that guarantees a faster and safer pharmacokinetic profile. These are also distant mimetics of highly active psychedelic structures, but are much more distinctive and have developed into complex nuclei with dual and multiple serotonin mimicry. The amide group, oxygen bridges, allyl and ethyl substituents, and methoxyl groups—almost all substituents have multiple readings—create a structure more akin to a multi-compartment train car, in which each car consists of two right-left gondolas, subtly intersecting. This behavior of the substance contributes to its multifaceted activity and high lipophilicity, as well as, possibly, simultaneous action on multiple receptors.



Row 16

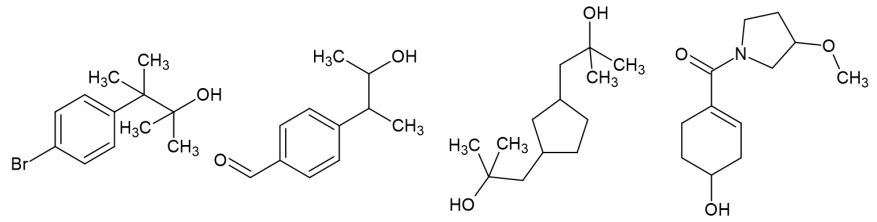
16.1 A highly lipophilic indole amine, similar to serotonin, psilocybin, and bufotenin. It has a 2-pentyl radical that reduces central activity (such radicals typically reduce psychoactivity to virtually zero), while simultaneously protecting the indole ring and enhancing bioavailability. The ethylamine group creates a relatively biolabile and non-polar accent, with limited pro-psychedelic potential. This is an attempt to allow the structure to penetrate deeper, avoid narcotic effects, and achieve correct pharmacokinetics, balancing between lipophilicity and a

short duration of action. This is what psilocybin should look like if it aspires to be used pharmacologically and safely.

16.2 The structure lacks an amino group, but instead features a subtle affinity accent of the double bond, which continues with a long lipophilic tail. The hydroxyl at the 4-position provides relative biostability. Lipophilic radicals with a long chain of 5-6 carbon atoms can, in some cases, provoke a slight affinity for 5-HT_2B receptors, which can subtly but synergistically reveal its potential.

16.3 Non-narcotic, highly lipophilic, a simple analogue of serotonin and psilocybin. The goal of the structure is to be extremely simple for research and safe for use, highly lipophilic, and highly available. Penetrating into neurons, into deep tissues, and the nucleus allows for a high safety profile and accurate pharmacokinetics.

16.4 Non-narcotic structural analogue of alphamethyl tryptamine and alphaethyl tryptamine. It has high lipophilicity and bioavailability, as well as a special radical at the 5-position, an allyl radical capable of carrying a lipophilic binding site in the inverse sense. This is an attempt to combine the simplicity of tryptamines with the multi-layered, subtle activity and lipophilicity of more pharmacologically complex structures.



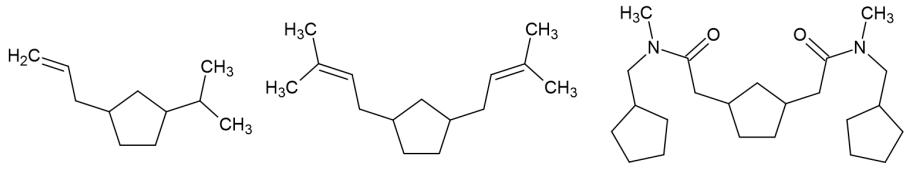
Row 17

17.1 An analogue of an outdated antidepressant with nootropic properties, presumably possessing neuroplastic potential due to relatively high activation of synaptogenesis and neurogenesis. The halogen in the para position (chlorine in the original drug) is a potent displacing agent, and the four methyl groups in the ethanolamine radical are protective radicals, which, together with the halogen, ensure the biostability of the structure. The displacing radical provokes pro-serotonergic activity; the substance is pharmacologically similar to tryptophols.

17.2 An attempt to eliminate the halogen and excess methyl groups; the substance is similar to the first in the line, but has the ability to form hydrophilic metabolites. This elimination pathway is safer and does not require halogenation of the aromatic ring or additional methyl groups in the framework.

17.3 Replacement of the aromatic ring with a pentane ring; a duplicate pro-ethylamine radical is used instead of the substituent. A substance with two reading vectors is not susceptible to the formation of toxic catabolites. Similar substances, closer to natural terpenes such as alpha-terpineol and menthol, can exhibit subtle effects and a high level of safety.

17.4 Pro-serotonin derivate of picrocrocin (the active ingredient in Saffron, *Crocus sativus*). This is an attempt to produce an alicyclic simple serotonin reuptake inhibitor with a pronounced lipophilic profile and potential for high neuroplasticity.



Row 18

18.1 A subtle, distant analog of carvacrol and arazone, in some ways pharmacologically close to the aforementioned substituted phenylethanols and tryptophols, sharing some similarities with erinacine. A minimalist synthetic terpene with good therapeutic potential and minimal toxicity risks.

18.2 A lipophilic dimeric version of the previous structure; the second radical not only acts as a displacer and duplicate pro-ethylamine but also completes the indole profile.

18.3 A combination of high-affinity psychedelic potency with the non-narcotic and subtle mimetic effects of the previous structures. High lipophilicity and bioavailability, extreme subtlety, but determined potency.

The library contains 52 compounds arranged in rows for convenient referencing during discussion and synthesis planning (e.g., "Compound 8.3" or "Row 14, second molecule"). Several intermediate tryptophol derivatives are also included as compromise structures between hydrophilic psilocybin and ultra-lipophilic erinacines.

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3. Predicted Advantages

- Synthesis 50–1000× cheaper and simpler than natural compounds (1–4 steps from commercial precursors)
- Superior blood-brain and intracellular barrier penetration (logP 4.4–6.8)
- Elimination of 5-HT_2B agonism → no valvulopathy risk
- Sustained NGF/BDNF induction without hallucinogenic effects
- Adjustable elimination half-life via lipophilicity tuning
- Potential telomerase activation and geroprotective properties
- High expected metabolic stability and low toxicity

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4. Conclusion

The presented analogues represent a new class of ultra-lipophilic, ultra-low-affinity "whisper" ligands capable of sustained neuroplastic and geroprotective effects. Rows 3–6, 8–10 and 14–16 appear especially promising. In silico evaluation and synthesis of top candidates are the logical next steps.

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